Appendix I3 – Advective Velocity Calculation

Objective

To evaluate the transport of the contaminants at Operable Unit (OU) 2 and assess the travel times from the different source areas, it is necessary to estimate the advective velocity in the shallow aquifer. Because the velocity (v) cannot be measured directly, it has to be calculated from the hydraulic gradient (i), hydraulic conductivity (K), effective porosity (n), and retardation factor (R). Some of these variables were estimated from in situ testing (K) and measurements (i), and some are taken from published literature (n, R). Because there is a range of plausible values for each of the input variables, a Monte Carlo (MC) type simulation is the preferred way for estimating the probable value of the advective velocity.

Major advantages of results from a MC simulation of velocity derive from two factors. First, establishing the range and distribution of input variables is a transparent process, based on a range of reasonably expected values, taken from the literature and a range of site-specific measures. Second, and perhaps even more important, the simulation generates a distribution of results which can be probabilitistically assessed. The following sections describe the methodology and results of the simulations.

Methodology

An MC modeling (e.g., Millard and Neerchal, 2001) in its simplest form consists of evaluating a model multiple times for input values that are drawn from probability distributions for each input variable in order to generate a probability distribution of the model outcomes. For the advective velocity calculation, the model is

$$v = \frac{\mathrm{Ki}}{\mathrm{nR}}$$

K has units of length/time (feet/day in this calculation) and the remaining variables are dimensionless.

K was estimated from slug tests and pumping tests on selected wells at OU2. K values estimated from pumping tests are typically higher than K values estimated from slug tests because during pumping, a larger zone of the heterogeneous aquifer material is hydraulically affected with more preferential groundwater flow pathways connected; this was indeed the case for OU2 aquifer testing results. Contaminant transport occurs primarily via the more permeable aquifer materials; therefore, the higher K values estimated from the pumping tests are more representative of the soils that the contamination migrated through. K is generally understood to be log-normally distributed in porous aquifer materials. However, the wells at OU2 were intentionally installed with screen intervals within coarse aquifer material, avoiding fine-grained units. Therefore, the pumping test results are characteristic of these coarse-grained units and are not expected to be log-normally distributed. The normality of the K distribution was tested by the Kolmogorov test; the K values from the pumping tests are neither normally nor log-normally distributed (Attachment 1). Because the probability distribution of K at OU2 could not be determined from the site data, the random K values for the MC simulation were drawn from a uniform distribution (i.e., each value of the variable has an equal probability of occurrence).

Additionally, an MC simulation was performed using a triangular distribution based on the minimum, maximum, and mean K values from the pumping tests (the mean K was assigned as mode in the triangular distribution). Both uniform and triangular distributions were also used for the remaining input variables.

The hydraulic gradient (i) was calculated from the difference between water level elevations at OW8A and MW30, and the distance between the two wells along the main contaminant transport pathway. Based on the historical water levels, the gradient does not change substantially across OU2, although overall water table fluctuates over time; the gradient magnitude does not deviate much from 0.0049 (Section 4 of the main text). A variation of ±10 percent in the gradient value was assumed for the MC simulations (the variation in the gradient measured across OU2 since August 2007 was less than ±5 percent). For the triangular distribution, the mode gradient value was assumed to be 0.0049.

The effective porosity values were not measured on site specific samples, because these measurements are biased for coarse grained soils due to the disruption of the sample during collection. Instead, the average of published values of minimum, maximum, and mean porosities for sands were used; that is, 0.1, 0.4, and 0.3, respectively (McWorter and Sunada, 1977). For the triangular distribution, the mode porosity value was assumed to be 0.3.

The retardation factor values were assumed to be between 1 (minimum possible R value) and 4. For the triangular distribution, the mode R value was assumed to be 2. The R value of 2 is a typical literature value; this value is considered conservatively high for the sandy materials at OU2 because of the expected low content of organic carbon in fluvial deposits and because of the similar extent of plumes of sorbing and non-sorbing compounds.

Two MC simulations were performed: one based on the uniform distribution of the input variable values and the second based on the triangular distribution. The input values for the calculation of v were drawn from the inverse cumulative probability distribution for each variable. A total of 10^6 evaluations were performed for each simulation.

A histogram and cumulative probability distribution were constructed from each simulation. The product of two (or more) normal (or uniform) distributions yields a distribution close to log-normal. The 50^{th} percentiles of cumulate results were determined from the computed cumulative probability distributions of the advective velocity values.

Results of Analysis

The results are presented in Figures 1 and 2 showing the probability density distributions and cumulative probability distributions for the two simulations, respectively.

Figure 2 displays the cumulative probability of the simulated advective velocity for each of the uniform and triangular input distributions. The centers of the distribution, the 50^{th} percentile of cumulate results are 1.69 and 1.71 feet per day or 616 and 623 feet per year (ft/y) for the uniform and triangular distributions, respectively; the 50^{th} percentiles represent the estimated most likely values of advective velocity at OU2. Figure 2 exhibits internally consistent best estimates, regardless of assumed input distribution, and indicates a broad range of possible velocities.

Omega Chemical Site Potentially Responsible Party (PRP) Organized Group's (OPOG's) letter to the National Remedy Review Board (NRRB) dated February 2, 2010, stated that estimated advective velocities are in the range of 160 to 250 ft/y. In light of the MC analysis, these values are at the extreme lower bound of the simulated advective velocity distributions, specifically at 8 and 16 percent, and 1.5 and 6 percent, for the uniform and triangular distributions, respectively.

Discussion

Based on the MC simulation results, the most probable value of the average advective velocity across OU2 is 616 to 623 ft/y. Because these values are very close, their average of 620 ft/y, is taken as the most probable advective velocity.

Additional hydraulic conductivity data could alter the estimated range of v values. Because the contaminant transport on the OU2 scale depends on large scale K distribution, larger (multi-well) scale pumping tests on wells screened in sandy units would be appropriate for the characterization of the relevant hydraulic properties. Larger scale pumping tests are known to yield higher K estimates than smaller scale tests; consequently, the estimated v value is expected to increase with further testing.

References

McWorter, D.B., and D.K. Sunada, (1977) Groundwater Hydrology and hydraulics, Water Resources Publications, Ft. Collins, CO.

Millard S. and N. Neerchal, 2001. Environmental Statistics with S-PLUS, Boca Raton, FL: CRC Press, 2001, ISBN 0-8493-7168-6, 830 pp.

Figure 1
Probability Density of Advective Velocity

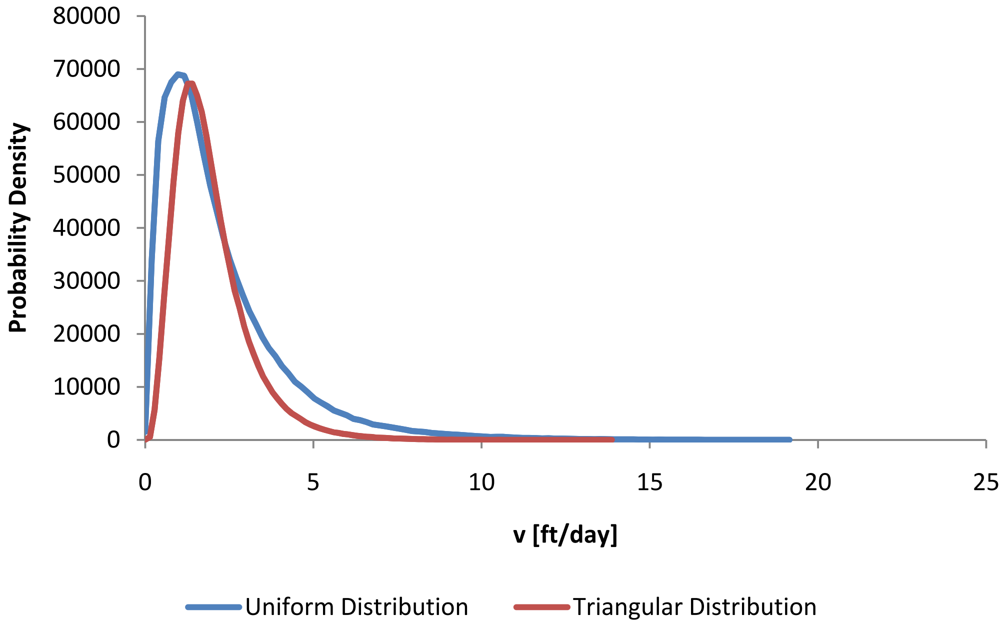
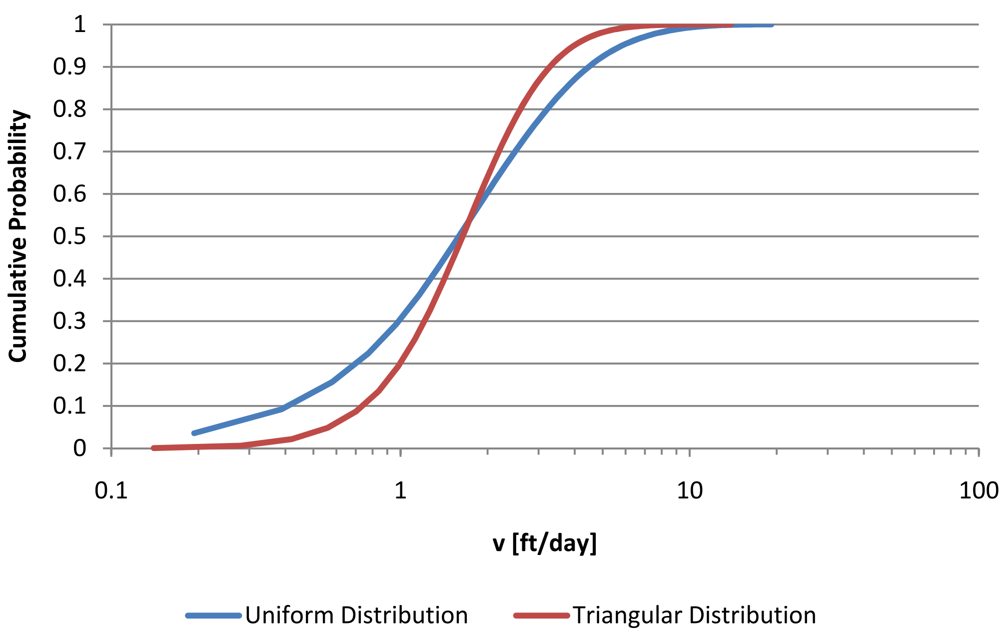


Figure 2
Cumulative Probability of Advective Velocity

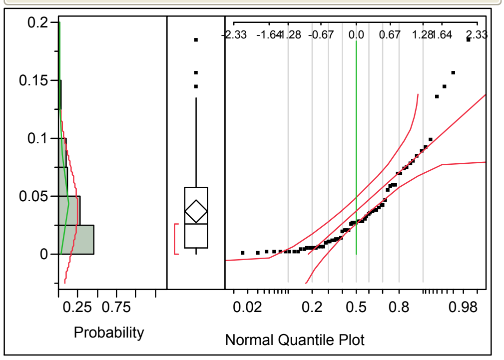


Attachment 1

Distribution test of K values, output from S-PLUS (Millard and Neerchal, 2001).

Distributions

ft_min



Normal(0.03715,0.0405)
LogNormal(-4.1005,1.55251)

Quantiles

100.0%	maximum	0.1832
99.5%		0.1832
97.5%		0.16444
90.0%		0.089
75.0%	quartile	0.05752
50.0%	median	0.02611
25.0%	quartile	0.00525
10.0%		0.00129
2.5%		0.00047
0.5%		0.00033
0.0%	minimum	0.00033

Moments

Mean	0.0371529
Std Dev	0.0405027
Std Err Mean	0.0049855
Upper 95% Mean	0.0471097
Lower 95% Mean	0.0271961
N	66

Fitted Normal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	μ	0.0371529	0.0271961	0.0471097
Dispersion	s	0.0405027	0.0345791	0.0488944

-2log(Likelihood) = -236.943081359319

Goodness-of-Fit Test

Shapiro-Wilk W Test

W	Prob<W
0.816302	<.0001*

Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.

Fitted LogNormal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Scale	μ	-4.100493	-4.480561	-3.720425
Shape	s	1.5525116	1.3210866	1.8603131

-2log(Likelihood) = -295.901848539043

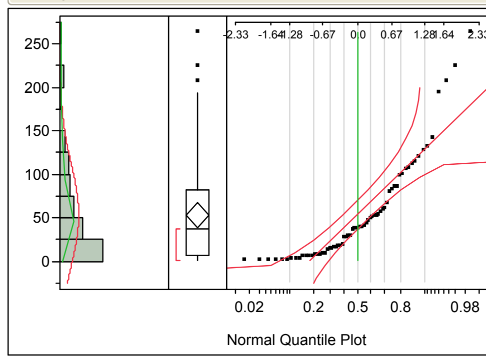
Goodness-of-Fit Test

Kolmogorov's D

D		Prob>D
0.153444	<	0.0100*

Note: Ho = The data is from the LogNormal distribution. Small p-values reject Ho.

ft_day



Normal(53.5002,58.3239)
LogNormal(3.17191,1.55251)

Quantiles

100.0%	maximum	263.808
99.5%		263.808
97.5%		236.786
90.0%		128.16
75.0%	quartile	82.8252
50.0%	median	37.5912
25.0%	quartile	7.55442
10.0%		1.85098
2.5%		0.67727
0.5%		0.468
0.0%	minimum	0.468

Moments

Mean	53.500196
Std Dev	58.323918
Std Err Mean	7.1791781
Upper 95% Mean	67.838004
Lower 95% Mean	39.162387
N	66

Fitted Normal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	μ	53.500196	39.162387	67.838004
Dispersion	s	58.323918	49.793951	70.407897

-2log(Likelihood) = 723.013506459927

Goodness-of-Fit Test

Shapiro-Wilk W Test

W	Prob<W
0.816302	<.0001*

Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.

Fitted LogNormal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Scale	μ	3.1719052	2.7918374	3.5519729
Shape	s	1.5525116	1.3210866	1.8603131

-2log(Likelihood) = 664.054739280203

Goodness-of-Fit Test

Kolmogorov's D

D		Prob>D
0.153444	<	0.0100*

Note: Ho = The data is from the LogNormal distribution. Small p-values reject Ho.